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31 Analysis of the Material Properties of Importance in the Classification of Toxicity of Graphene Nanomaterials.

Jenny R. Roberts, Vamsi K. Kodali, Aleksandr B. Stefaniak, Theresa E. Boots National Insititute for Occupational Safety and Health, Morgantown, USA

Graphene (Gr) nanomaterials are one of the fastest growing nanotechnology markets with a variety of applications in numerous industries due to a battery of unique physicochemical properties related to two-dimensional structure. Occupational exposure to graphenes by inhalation is a concern. Understanding the relationship of these properties to toxicity is critical for better predicting risk. The goal of this study was to associate material properties of this class of two-dimensional material with parameters of pulmonary toxicity and pathology. In vivo pulmonary exposure studies were previously conducted to compare different graphene nanomaterials [Gr that varied in lateral dimension, graphene oxide (GO), and reduced GO (rGO)] and carbon-based reference nanomaterials [carbon black (CB) and multi-walled carbon nanotubes (MWCNT)]. Size, density, surface area, oxygen content, as well as reactivity, agglomeration size, and zeta potential in delivery vehicle for oropharyngeal aspiration were measured. MWCNT and rGO caused persistent inflammation and a fibrotic response over time whereas inflammatory responses to other materials were transient. A classification Random Forest was used to predict toxicity grouping based on material properties to determine variable importance. Grouping was determined by significant difference from control using lavage and pathology outcomes and incidence. Toxicity ranking was MWCNT=rGO>>Gr5=Gr20=GO=CB≥Gr1. Variable of importance varied by time and toxicity parameter; however, density and mean agglomerate size were critical factors in the highly toxic materials whereas surface area was the most important factor in less toxic groups. This study contributes to understanding the structure-activity of this material class and read-across toxicity assessments of similar emerging materials.